1,5-Dihydroxynaphthalene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 152 °C

Global applicability domain: Inside

Local applicability domain index: 8.64e-01

Confidence level: 5.84e-01

Nearest Neighbors from the Training Set

Image not found
Naphthalene-1,7-diol
Measured: 181
Predicted: 165

Image not found
Naphthalene-1,6-diol
Measured: 138
Predicted: 162

Image not found
1,3-Naphthalenediol
Measured: 124
Predicted: 159

Image not found
Biphenyl-2,5-diol
Measured: 103
Predicted: 117

Image not found
2,6-Naphthalenediol
Measured: 220
Predicted: 185